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A study of the effects of disorder in the 2D Hubbard model

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Title: A study of the effects of disorder in the 2D Hubbard model

We study the effects of disorder on long range antiferromagnetic correlations and the Mott gap in the half-filled, two dimensional, repulsive Hubbard model. We employ Hartree-Fock (HF) and Quantum Monte Carlo (QMC) techniques in our study of the bond and site disordered models. Results from mean field (HF) calculations are used to develop a qualitative picture of the physics and to guide our choice for input to the QMC methods. The basic properties of two QMC methods for correlated fermions are discussed, and the results from these different approaches are presented. This work was performed under the auspices of the U.S. Department of Energy by the University of California and Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

A study of the effects of disorder in the 2D Hubbard model

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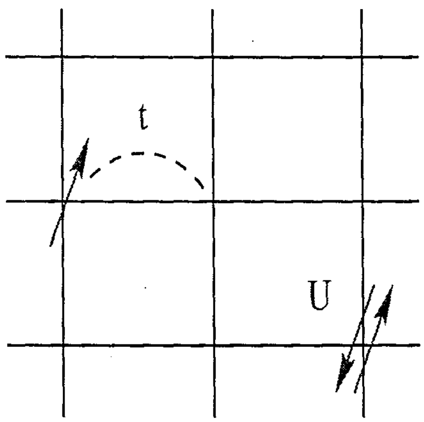
Introduction

- Main Goal: To study correlated Fermi systems in the presence of disorder. We will consider model systems with hopping and on–site disorder. Our focus is the destruction AFLRO and the behavior of the Mott gap in the presence of disorder.
- The single band $2D$ Hubbard model, it encapsulates many of the most interesting qualitative many body effects. It is also one of the simplest correlated models to work with.
  - The possibility of interacting fermions to order.
  - The appearance of insultating states in systems with partially filled bands.
  - $U < 0$, superconductivity.
  - $U > 0$, model for Metal–Insulator.
  - Boson Hubbard - a model for a supersolid.
  - $1D$ model is solved exactly by Bethe ansatz, an insulator for all $U > 0$, no MIT.
  - In infinite dimensions variants of the HM can be solved exactly, (Dynamical Mean Field Theory)
  - No solution for $1 < d < \infty$. Many approaches are employed for finite dimensions: MFT, QMC, RG, PT, ...
- We employ several techniques in our study:
  - Exact diagonalization of the non-interacting disordered model.
  - Restricted Hartree–Fock (rHF).
  - Unrestricted Hartree–Fock (uHF).
  - Determinant Quantum Monte Carlo (DQMC): R. Blankenbecler et al., PRD **24,** 2278 (1981).
  - Constrained Path Quantum Monte Carlo, (CPQMC): S. Zhang et al., PRL **74,** 3652 (1995).

Hubbard Model

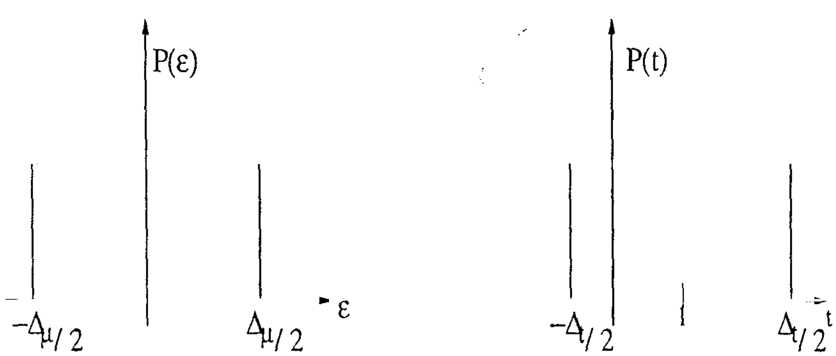
$$H = - \sum_{<i,j>,\sigma} t_{i,j}(c^\dagger_{i\sigma}c_{j\sigma} + c^\dagger_{j\sigma}c_{i\sigma}) + U\sum_i (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)$$
$$+ \sum_i (\epsilon_i - \mu)(n_{i\uparrow} + n_{i\downarrow})$$



Nearest neighbor hopping

On–site repulsion

- $c_{i\sigma}(c^\dagger_{i\sigma})$, creation (annihilation) operators for fermions of spin σ
- $t_{i,j}$ random hopping matrix
- U, on–site repulsion
- ϵ_i random site energy, μ chemical potential ($\mu = 0$, 1/2 filling)
- We will consider systems with uniform, uncorrelated disorder:



Mean Field Treatment

Develop a qualitative picture of the $2D$ disordered phase diagram. A mean field decomposition of the Hubbard model,

$$n_{\mathbf{i}\sigma} \to \langle n_{\mathbf{i}\sigma}\rangle + \delta n_{\mathbf{i}\sigma},$$

where

$$\delta n_{\mathbf{i}\sigma} = n_{\mathbf{i}\sigma} - \langle n_{\mathbf{i}\sigma}\rangle.$$

produces two independent Hamiltonians

$$H = H_\uparrow + H_\downarrow - U\sum_{\mathbf{i}}\langle n_{\mathbf{i}\uparrow}\rangle\langle n_{\mathbf{i}\downarrow}\rangle - (U/2+\mu)\sum_{\mathbf{i}\sigma} n_{\mathbf{i}\sigma} + UN/4$$

$$H_\sigma = -\sum_{\langle \mathbf{i},\mathbf{j}\rangle} t_{\mathbf{ij}}(c^\dagger_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} + c^\dagger_{\mathbf{j}\sigma}c_{\mathbf{i}\sigma}) + \sum_{\mathbf{i}}\left[U\langle n_{\mathbf{i}\acute{\sigma}}\rangle + \epsilon_{\mathbf{i}}\right] n_{\mathbf{i}\sigma}$$

Two mean field treatments:

rHF: Use the ansatz $\langle n_{\mathbf{i}\sigma}\rangle = (n + \sigma(-1)^{\mathbf{i}}m)/2$, solve the resulting equations by exact diagonalization.

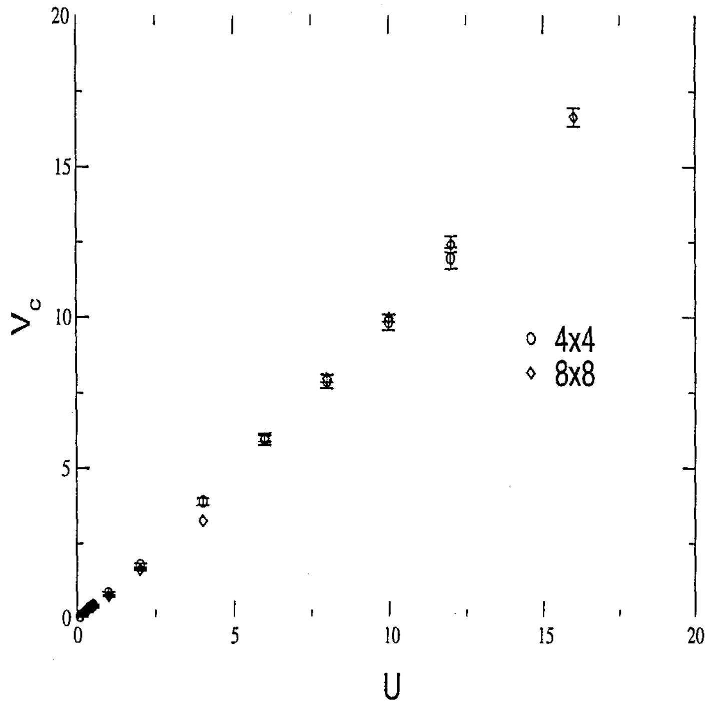
uHF: $\langle n_{\mathbf{i}\sigma}\rangle$ can vary in an arbitrary manner. One solve H self–consistently.

Observables:

- Staggered magnetization: $M_s = 1/N\sum_{i=1}^{N}(-1)^i m_i$, where m_i is the magnetization at site i.
- Local magnetization: $M_l = 1/N\sum_{i=1}^{N}|m_i|$.
- Compressibility: $\kappa = \frac{1}{N}\partial\langle n\rangle/\partial\epsilon = \frac{\beta}{N}(\langle N^2\rangle - \langle N\rangle^2)$
- Inverse participation ratio: $R^{-1} = 1/N\sum_{n,i}|\psi_i^n|^4$, where the sum is over all states (n) and sites (i).

rHF Results

Phase–diagram for on–site disorder



A near linear relationship between V_c and U.

rHF equations:

$$H = H_{\uparrow} + H_{\downarrow} - \mu \sum_{\mathrm{i},\sigma} n_{\mathrm{i}\sigma} + (Un/2 - U/2) \sum_{\mathrm{i},\sigma} n_{\mathrm{i}\sigma} + UN(m^2 - n^2)/4$$

$$H_{\sigma} = -\sum_{\langle \mathrm{i},\mathrm{j} \rangle} t_{\mathrm{i},\mathrm{j}} (c^{\dagger}_{\mathrm{i}\sigma} c_{\mathrm{j}\sigma} + c^{\dagger}_{\mathrm{j}\sigma} c_{\mathrm{i}\sigma}) + \sum_i (\epsilon_{\mathrm{i}} + \acute{\sigma}(-1)^i Um/2) n_{\mathrm{i}\sigma}$$

Solve $H_{\uparrow}$ and $H_{\downarrow}$ by ED.

uHF Results

Procedure:

$$H = H_\uparrow + H_\downarrow - U\sum_{\mathrm{i}}\langle n_{\mathrm{i}\uparrow}\rangle\langle n_{\mathrm{i}\downarrow}\rangle$$

$$H_\sigma = -\sum_{\langle \mathrm{i,j}\rangle} t_{\mathrm{ij}}(c^\dagger_{\mathrm{i}\sigma}c_{\mathrm{j}\sigma} + c^\dagger_{\mathrm{j}\sigma}c_{\mathrm{i}\sigma}) + \sum_{\mathrm{i}}\left[U\langle n_{\mathrm{i}\acute{\sigma}}\rangle + \epsilon_{\mathrm{i}}\right] n_{\mathrm{i}\sigma}$$

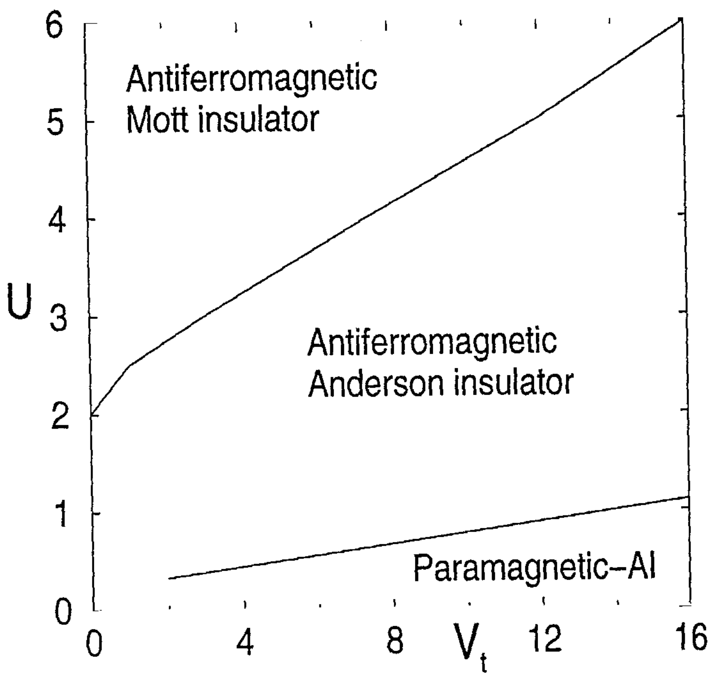
1. Choose a disorder realization, $t_{i,j}$ or ϵ_i.
2. Choose an initial mean occupation, $\langle n_{i\sigma}\rangle$.
3. Diagonalize the two Hamiltonians, $H_\uparrow$ and $H_\downarrow$.
4. Form a new mean occupation distribution, $\langle n_{i\sigma}\rangle$.
5. Substitute the new $\langle n_{i\sigma}\rangle$ into the Hamiltonian.
6. Iterate steps 3-5 to self–consistency.
7. Measure observables.
8. Repeat steps 2-7 with a different initial condition. Test for convergence of physical quantities.
9. Repeat steps 1-8 for a different disorder realization.

Results:

- The same three phases are observed for the two types of disorder.
- The system always remains and insulator.

uHF Results

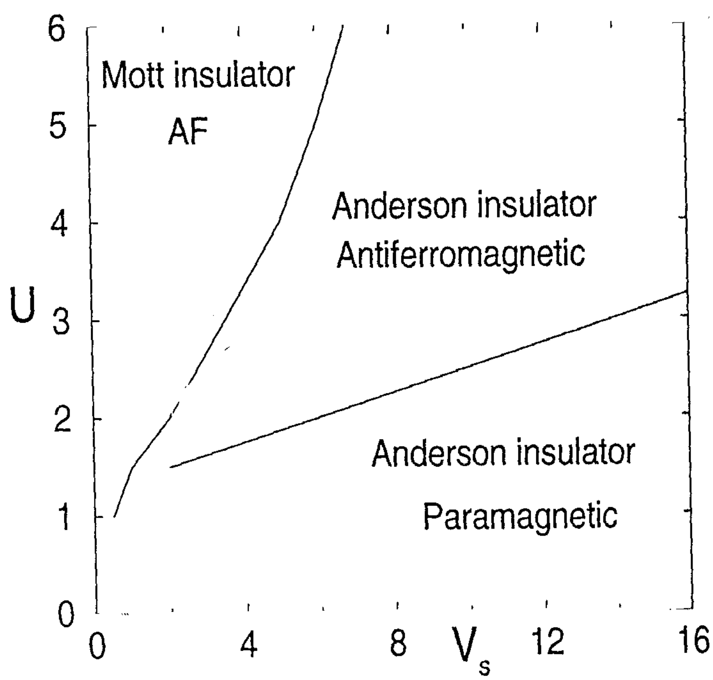
Hopping Disorder ($N = 36, 64, 100$)



$M_l = M_s$ always, no spin glass

$R^{-1} \neq 0$, always an insulator

On–Site Disorder ($N = 36, 64, 100, 144$)



AFMI

$M_s \neq 0$
$\kappa = 0$

AFAI

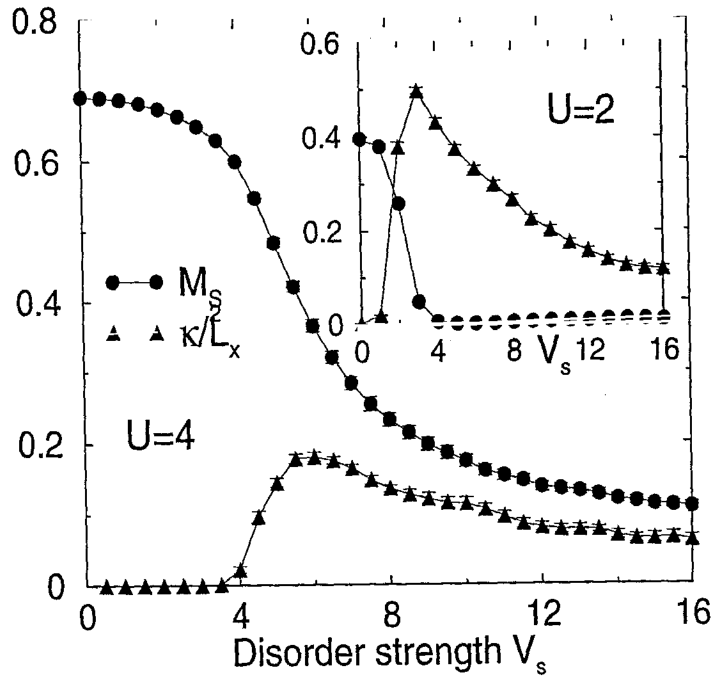
$M_s \neq 0$
$\kappa \neq 0$

PMAI

$M_s = 0$
$\kappa \neq 0$

Note: At $U = 4$, disorder does not destroy AFLRO.

uHF Results



Evolution of the staggered magnetization and compressibility with on–site disorder

12×12 lattice

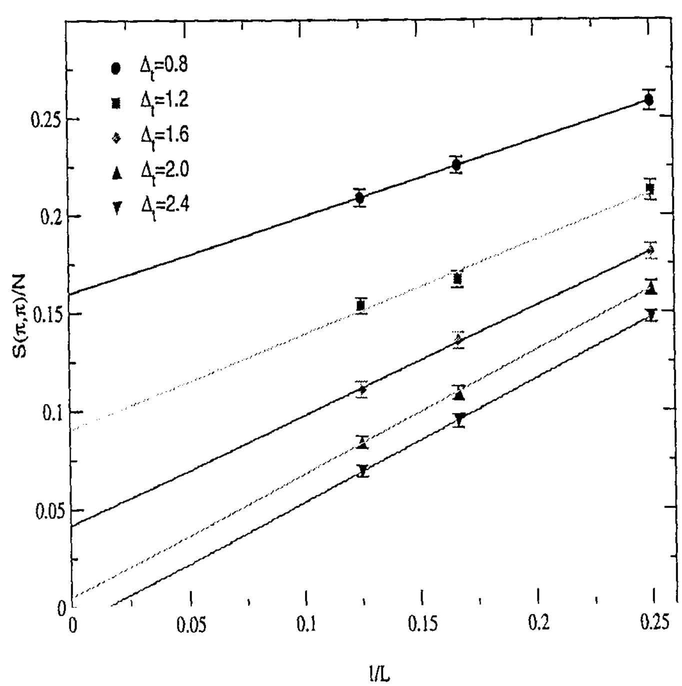
Disorder destroys magnetic order for $U = 2$ but not for $U = 4$

CPQMC Results

The CPQMC algorithm:

- $|\Psi^{(n+1)}\rangle = \exp^{-\Delta\tau H}|\Psi^{(n)}\rangle$
- $|\Psi^{(n)}\rangle = \sum_k c_k^{(n)}|\phi_k^{(n)}\rangle$, Slater determinant basis.
- $|\Psi_T\rangle$, trial wave function.
- $\langle\Psi_T|\phi_k^{(n)}\rangle \neq 0$, constraint.
- The method ($T = 0$) allows for investigations of the Hubbard model in regions where there is a sign problem. This is an issue for the case of on–site disorder.
- In our calculations, $|\Psi_T\rangle$ is a disorder unrestricted Hartree–Fock state with $U = 0.5$.

Hopping Disorder



Spin Wave Theory:
Huse PRB **37**,2380(1988)
$S(\pi,\pi)/N = M^2/3 + O(L^{-1})$

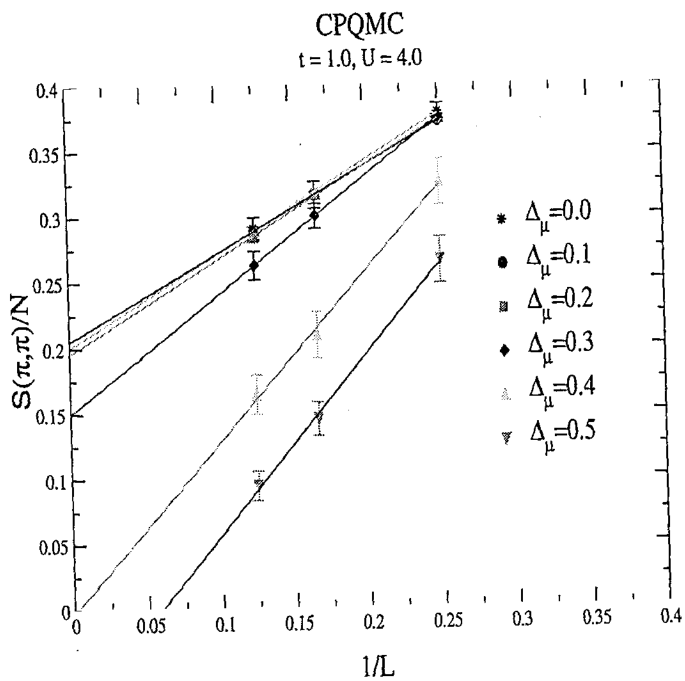
Critical disorder
$V_c \approx 2.1$

Compare to DQMC result,
Ulmke et al. PRB **55**,4149(1997)

$V_c \approx 1.6$

CPQMC Results

On–site Disorder



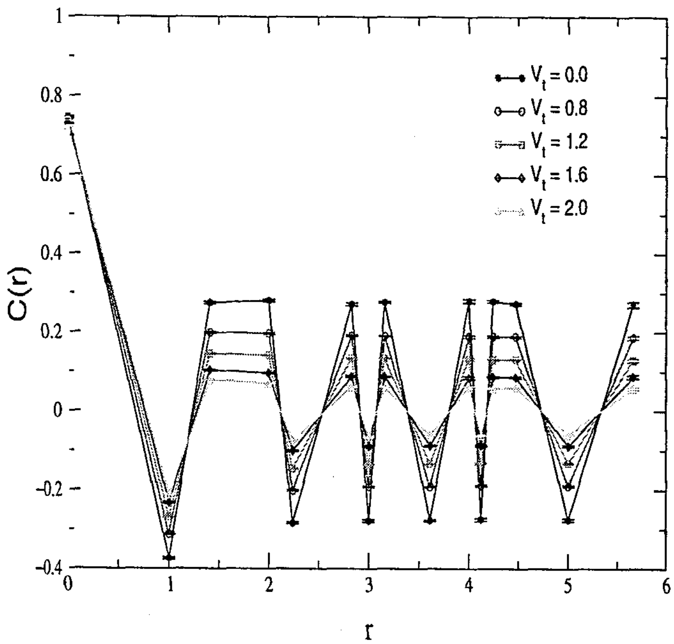
Critical Disorder:

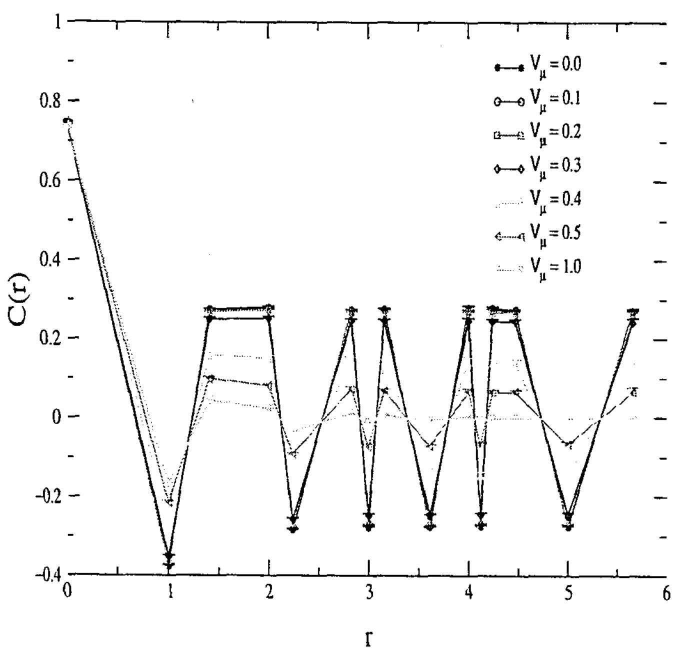
$V_c < 0.4$

No DQMC or analytic data available for comparison.

CPQMC Results

Correlations





Summary

- In the mean field limit, unrestricted Hartree–Fock, the disordered Hubbard model is an insulator. At appreciable interaction strengths, disorder does not destroy AFLRO. These results hold for hopping and on–site disorder.
- Monte Carlo simulations at $U = 4$ show a loss of AFLRO with increased disorder.
- Preliminary results from CPQMC yield $V_c \approx 2.1$ for the case of hopping disorder. This result is in reasonable agreement with that obtained via DQMC, $V_c \approx 1.6$.
- Preliminary results for on–site disorder indicate that the $V_c \leq 0.4$. The enhanced ability to form on–site pairs rapidly destroys AFLRO.

Future Plans

- Need to study the effect of the trial wave function on our results; the extrapolated values for staggered magnetization are high.
- Complete work on the critical disorder at $U = 4$.
- Study the effect of the interaction strength U on the half–filled model.
- Map out the ground state phase diagram as a function of V and U.